CompassCDS
Hydrocarbon Reporting Tool
User Guide

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Contents

Overview....3

Definition of Terms....5

Report Layout....6

- Logo....6
- Report Header....6
- Page Header....6
- Component Table....7
- Calculations Table....7
- Extended Reporting....7
- Report Footer....7

Installation....8

Configuration....8

- General....8
- Headers....8
- Report....9
- Extended Reporting....9
- Export....9

Troubleshooting....10

Sample Report Output....11

Standard Methods and Calculations....12

Appendix A: Peak results from CDS....14

Appendix B: Physical Constants....14

Appendix C: Report Families and Temperatures for Components....14

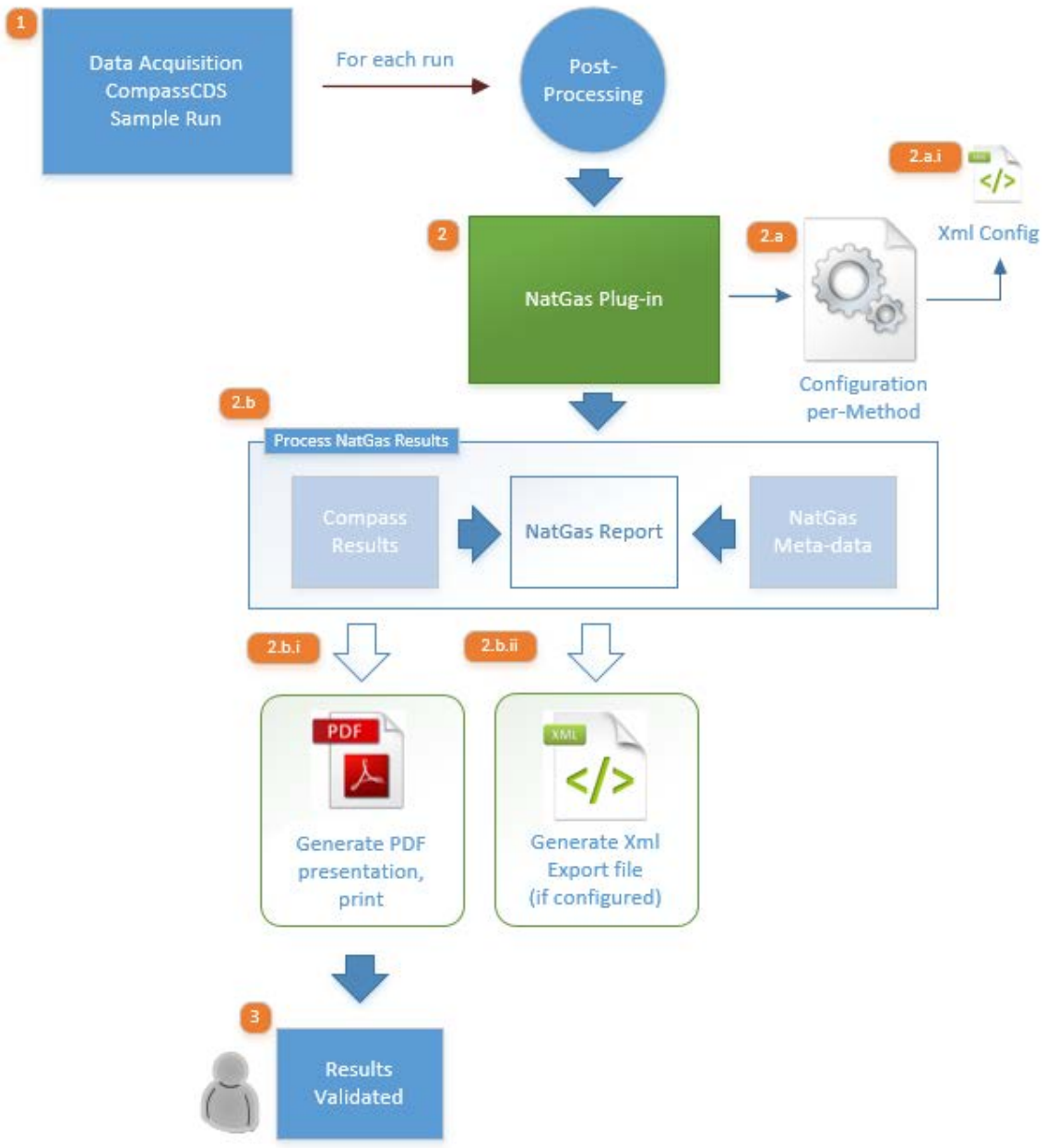
Appendix D: Report Families and Pressure for Calculations....15

Appendix E: IS0 6976 Natural Gas – Calculation of Calorific Values, Density, Relative Density and Wobbe Index from Composition....16

Overview

The Hydrocarbon Reporting Tool is a program that runs within the CDS (Chromatography Data System) Plug-in architecture. Meaning, the program is configured and launched via the CDS post-processing section, and the program leverages functionality exposed by rich CDS API's. As a Plug-in, the Tool provides specific Hydrocarbon Reporting as an extension of the CDS.

The Tool employs industry-standard Xml-based Report Definition Language (RDLC). RDLC used to create the report is generated dynamically based on report configuration and CDS results. The final output is Portable Document Format (PDF) and is viewed using industry-standard Adobe Acrobat Reader.

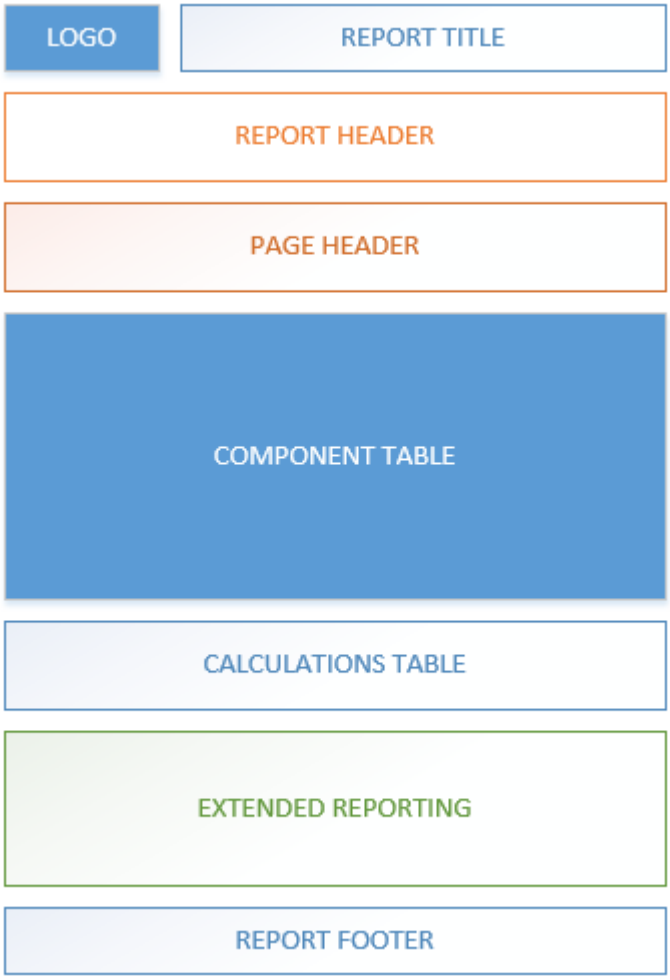


1. Data Acquisition – The Instrument controlled by CompassCDS performs the analysis on the sample, during which the raw data acquisition takes place. CompassCDS processes results and stores all data in a local .DATA files. This data includes raw data points, control method, and calculated results for each detector.
2. Post-Processing – At the end of each Run the post-processing takes place. The Hydrocarbon Reporting (NatGas) plugin is run.
    a. Each CompassCDS Method must be configured in the post-processing section. Using the Settings Dialog, the user may configure exactly how the report and associated output will be produced. For example, GPA-2177 includes specific components, calculations, and C7+ extended reporting. These will be selected within the Settings dialog for each Method.
        - Of the elements selected for a report, the user may further specify which components, values, and calculations will be included in the Xml export. All settings are stored in a method-specific local Xml file. This provides portability of settings.
    b. Processing NatGas – The plugin processes CompassCDS results and produces the NatGas Report using meta-data which defines the Components and Calculations. The output of the NatGas Report is a PDF file and Xml export of the data.
        - A PDF file is generated which can be viewed by the user to verify results. The PDF rendering of the NatGas report includes all peak data plus NatGas calculations. The PDF report may be printed automatically. The PDF file is stored in a configured location.
        - The Xml export file is produced as part of the post-run NatGas processing. The user may control exactly which data gets exported from the Settings dialog. The Xml export file is used downstream to write NatGas results to CompassDB. The Xml export file is stored in a configured location.
3. Results Validation – The Analyst may verify the correctness of each run. They may view the chromatogram within the CompassCDS UI, or use the NatGas PDF output.

Definition of Terms

Peak Results	Values generated by CDS during the run which represent the results of the analysis. Refer to Appendix A.
Physical Constants	Properties of each component, these values are fixed (not calculated). Physical constants are used by the reporting engine to produce calculations and can also be used as columns in the Component Table. See Appendix B.
Components	A complete list of components is contained in the reporting database. If used in the report, the Component Name must match the CDS component name from the method. The reporting database contains a set of components for each reporting family (GPA, ASTM, ISO), and within a family, a set of Components by Temperature (See Appendix C). Each Component is also assigned a Carbon Number which is used in Calculations and Extended Reporting. There are over 200 Components configured for each Family/Temperature combination.
Calculations	Calculations are the heart of the Hydrocarbon Reporting Tool. The reporting engine uses a Peak Results, Physical Constants and a Formula to generate values. Some calculations are performed at the Component level and may be selected as columns in the Component Table. Other Calculations are total computed values based on overall results of the analysis. These components can be selected to appear in the Calculations Table section of the report. The reporting database contains a set of Calculations for each Reporting Family, and within each Family by Pressure. Refer to Appendix D.

Report Layout



Logo

The Logo area contains an image that is 240 X 70 pixels. The program uses any file named “logo.jpg” found in the install folder, so it’s possible to change the logo by just swapping out the image file. The Logo is not configured within the Settings dialog.

Report Header

The Report Header appears on top of the first page of the report output. It is controlled by the Settings dialog as a list of selected items from available Channel (Global) Variables.

Page Header

The Page Header appears on top of each page of the report output. It is controlled by the Settings dialog as a list of selected items from available Channel (Global) Variables.

Component Table

The Component Table contains a list of all configured components, with each row in the table a single component. Rows and Columns in the Component Table are configured in the Settings dialog. The columns in the table may be sourced from one of the following:

1. The actual Peak results from CompassCDS (QTY, AREA, AREAP, RT).
2. Calculations performed by the reporting engine using CDS results, Physical Constants and static values (Summ Factor, C*n*+, Saturation, etc.)

Calculations Table

The Calculations Table contains a list of Calculations supported by the reporting engine, and their values. Calculations are configured using the Settings dialog. Calculations tables may be split out by Pressure, resulting in separate report grouping sections for each Pressure and selected Calculations.

Extended Reporting

Extended Reporting provides a means to group Components based on Carbon No. Sets of components are grouped in this section with a subtotal. At the end of the section a combined total is calculated. Extended Reporting Components and Columns are configured using the Settings dialog. Only Components with Carbon No greater than zero are available for selection. CDS Results, Physical Constants and Calculation-based Columns are available for selection. Certain Calculations are designed specifically for Extended Reporting.

Report Footer

The Report Footer appears at the bottom of each page and contains the date/time of the report generation in the lower-left corner, and the page number in the right corner.

Installation

Installation Steps:

1. Copy the installer files (setup.exe, HydrocarbonReportSetup*.msi) to a temporary location.
2. Launch the installer by double-clicking the setup.exe program.
3. Accept the defaults for Installation Folder and Allow Everyone access.
4. Note: It is strongly recommended the Hydrocarbon Reporting Plugin be installed in the default folder.
5. Click Next to confirm.
6. The Hydrocarbon Reporting Tool is installed, you may exit the dialog. The Plugin may now be configured in the post-run section of the Chromatography Data System.

Configuration

Each Method using the Hydrocarbon Reporting Tool must be configured using the Settings dialog. Once launched the user has access to the following sections:

General

Report Name – The title that appears on the top of the PDF report.

Output Folder – The folder where PDF reports are written at the end of each run. NOTE: User must have write access to the folder,

Static File Name – May use a CDS variable name for the name of the PDF output. Using this, any file named the same is overwritten.

Show Report in Viewer – Launches the PDF viewer (Adobe Reader) after the PDF output is generated.

Automatically Print Report – When checked, will print the PDF output automatically to the configured default printer on the users' workstation.

Headers

The user may configure headers by selecting from a list of global CDS variable names. Defaults are provided.

Report Header – appears at the top of the first page.

Page Header – appears at the top of each page. A maximum of 5 selections is allowed.

Report

Family and Temperature – Selects the reporting family and temperature. See Appendix C

Liquid / Gas - specifies which Calculations are available (Summary Calculations Tab).

Component Table

Pressure – specifies the Pressure Base used in Hydrocarbon Reporting calculations. Refer to Appendix D.

Search – User may search list of available Components by typing in part of the component name, the program recognizes each keystroke.

Components – user may select from a list of available Components, defaults are provided. This selection is the basis of the Component Table section of the report. The Component names are derived from metadata. CDS Peaks configured in the Method must name-match exactly these Component names. Selected Components may be re-ordered using the up/down arrows.

Columns – this selection identifies the columns found in the Component Table section of the report. User selects from a list of available peak-level CDS results, Physical Constants and Calculations. Defaults are provided. Selected columns may be re-ordered using the up/down arrows.

Summary Calculations

Pressure – specifies the Pressure Base used in Hydrocarbon Reporting calculations for Summary Calculations. The default is based on the selected pressure base for the Component Table.

User may select from a list of available Summary Calculations. These are derived from Hydrocarbon Reporting metadata. It is possible to report Calculations at one or more pressure bases, this is done by selecting another Pressure, and building the tree-view of selected Pressure and Summary Calculations. This results in separate tables created in PDF output.

Selected calculations may be re-ordered using the up/down arrows.

Extended Reporting

Search – User may search list of available Components by typing in part of the component name, the program recognizes each keystroke.

Available Components are listed with Carbon Number in parenthesis. Extended tables are built be selecting one or more components with the same carbon number. A new table is built in report output for each configured Carbon Number. A tree-view is used to represent how the report output will be organized. Defaults are not provided.

Columns – this selection identifies the columns found in the Extended Table section of the report. User selects from a list of available peak-level CDS results, Physical Constants and Calculations. Defaults are provided. Selected columns may be re-ordered using the up/down arrows

Export

Hydrocarbon Report output generated each run may be saved to XML by selecting the checkbox. The folder for the Xml export must be selected. Users may select elements from any of the Hydrocarbon Report sections. Default selections are made.

Troubleshooting

Problem	Solution
The plug-in does not appear in the post-processing section of the CDS.	Ensure the Plug-in is installed and registered with the CDS correctly. If necessary contact support channels.
The software license displays DEMO USE ONLY	A valid license key must be provided to the customer and placed in the install folder.
ERROR: *Method not specified* when launching the Settings dialog.	The Hydrocarbon Reporting Tool is not able to locate the CDS Method which is required for configuration.
Component Table values (columns) are zero.	Ensure the CDS is configured to detect a Peak with the same name. Components are name-matched between CDS peak definition and Hydrocarbon Reporting metadata.
Report PDF output not found	Check the output folder configured in the General section for newly created PDF files. Ensure the logged-in user has access to the configured output folder. If the files are not being created this could indicate a General Failure.
General failure	A general failure to produce the report could be due to various conditions. Click the View Log button from the Settings dialog and view the logs starting at the end of the file. If no reasonable explanation is clear from the logs then proceed to contact support channels.

Sample Report Output

Hydrocarbon Reporting Solutions

Hydrocarbon Reporting

User Name:	Administrator	#Vial:	1
System Name:	GPA 2286	Inj. Vol.:	0.000
Acquisition Date & Time:	7/27/2015 4:24:25 PM	Method Name:	GPA 2286
Multiplier:	1.000	Divisor:	1.000

Component Results (14.65)

Name	Quantity [Mol%]	Time [Min]	Area [uV.Min]	Qty (Norm) [Mol %]	Heating Value (Dry I	Heating Value (Dry	MW Fraction	Relative Density (G)	GPM	Liquid Volume Fra
methane	72.5990	0.20	15.30	76.1475	769.089	769.484	12.22	0.22844	12.88	0.42
ethane	8.9830	0.40	3.46	9.4221	166.742	166.828	2.83	0.03357	2.51	0.12
propane	6.0230	0.50	3.28	6.3174	158.952	159.033	2.79	0.03204	1.74	0.16
n-butane	3.1780	0.70	2.08	3.3333	108.743	108.799	1.94	0.01947	1.05	0.13
n-pentane	0.9440	0.90	0.68	0.9901	39.692	39.712	0.71	0.00624	0.36	0.05
carbon dioxide	1.0250	0.30	1.35	1.0751	0.000	0.000	0.47	0.00879	0.18	0.04
nitrogen	2.5880	0.10	3.45	2.7145	0.000	0.000	0.76	0.02190	0.30	0.07
	95.3400		29.60	100.0000	1243.219	1243.856	21.72		19.02	1.00

Calculations at Pressure Base 14.65

Heating Value (Dry Ideal) Total BTU:	1243.219	Heating Value (Dry Real) Total BTU:	1243.856
Component MW Total :	21.72	Relative Density (Water = 1.0) Total :	0.350
Summation Factor (Sat) Total :	0.01549	Heating Value (Sat Ideal) Total BTU:	1221.462

Extended Reporting

C4

Name	Quantity [Mol%]	Time [Min]	Area [uV.Min]	Area [Norm]	Molecular Weight	Summation Factor	Z Factor
isobutane	0.0000	0.00	0.00	0.0	58.12	0.04	0.17
n-butane	3.1780	0.70	2.08	6.3	58.12	0.05	0.18
Subtotal:	3.1780		2.08	6.3	116.24	0.09	0.35

C5

Name	Quantity [Mol%]	Time [Min]	Area [uV.Min]	Area [Norm]	Molecular Weight	Summation Factor	Z Factor
isopentane	0.0000	0.00	0.00	0.0	72.15	0.06	0.22
n-pentane	0.9440	0.90	0.68	2.1	72.15	0.06	0.23
Subtotal:	0.9440		0.68	2.1	144.30	0.12	0.45
Total:	4.1220		2.76	8.4	260.54	0.21	0.80

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Standard Methods and Calculations

The Hydrocarbon Reporting Tool will use formulae and report results based on the following international standard tables and methods.

IS0-6796 Natural Gas – Calculation of calorific values, density, relative density and Wobbe index from composition

GPA 2145-09 Table of Physical Properties for Hydrocarbons and Other Compounds of Interest to the Natural Gas Industry

GPA 2172-09 Calculation of Gross Heating Value, Relative Density, Compressibility and Theoretical Hydrocarbon Liquid Content for Natural Gas Mixtures for Custody Transfer

GPA 2286-95 Tentative Method of Extended Analysis for Natural Gas and Similar Gaseous Mixtures by Temperature Programmed Gas Chromatography

GPA 2186-02 Method for the Extended Analysis of Hydrocarbon Liquid Mixtures Containing Nitrogen and Carbon Dioxide by Temperature Programmable Gas Chromatography

GPA 2261-00 Analysis for Natural Gas and Similar Gaseous Mixtures by Gas Chromatography

ASTM D 3588-98 (2011) Standard Practice for Calculating Heating Value, Compressibility Factor, and Relative Density of Gaseous Fuels

Calculations common to the above mentioned standard methods may include:

- Component Mol %, Normalized Component Mol %, GPM (Gallons per 1000 ft^3)
- Fraction Molecular Weight, Specific Gravity, Compressibility
- Ideal Relative Gas Density, Ideal Gas Density, Real Relative Gas Density, Real Gas Density
- Heating Value $kJ.mol^{-1}$ (Superior), Heating Value $kJ.mol^{-1}$(Inferior), Heating Value $MJ.kg^{-1}$ (Superior), Heating Value $MJ.kg^{-1}$ (Inferior)
- Heating Value $MJ.m^3$ (Superior), Heating Value $Mj.m^3$ (Inferior), Gross Heating Value BTU/ft^3 (Ideal)

Dry Gas

- Net Heating Value BTU/ft^3 (Real) Dry Gas, Gross Heating Value BTU/ft^3 (Ideal) Saturated gas
- Net Heating Value BTU/ft^3 (Real) Saturated gas, GPM C2+, GPM C3+, GPM C4+
- Wobbe Index, Research Octane Number (RON), Motor Octane Number (MON), Carbon Number.

A complete list of required individual component and total calculations follow.

The values mentioned above are to be reported at different temperature and pressure bases that include:

- ISO 6976 (0-0 ºC).cfg Similar to the ISO Default configuration except the physical property data are for a combustion temperature of 0 ºC and a metering temperature of 0 ºC.
- ISO 6976 (15-0 ºC).cfg Similar to the ISO Default configuration except the physical property data are for a combustion temperature of 15 ºC and a metering temperature of 0 ºC.
- ISO 6976 (25-0 ºC).cfg Similar to the ISO Default configuration except the physical property data are for a combustion temperature of 25 ºC and a metering temperature of 0 ºC.
- ISO 6976 Default (15-15 ºC).cfg Identical to the ISO Default configuration with the physical property data for a combustion temperature of 15 ºC and a metering temperature of 15 ºC.
- ISO 6976 (20-20 ºC).cfg Similar to the ISO Default configuration except the physical property data are for a combustion temperature of 20 ºC and a metering temperature of 20 ºC.
- ISO 6976 (25-20 ºC).cfg Similar to the ISO Default configuration except the physical property data are for a combustion temperature of 25 ºC and a metering temperature of 20 ºC.

The pressure base for all the above ISO-6976 calculations is 101.325 kPa

- GPA 2172, 2186, 2286 and 2261 at 14.696 psia, 14.650 psia and 14.730 psia at 60 º F and 76 º F for Dry, with options for Wet and Saturated calculations
- ASTM 3588 14.696 psia at 60 º F

Appendix A: Peak Results from CDS

Name	Identifier	Total	Format
Name	NAME	FALSE	
Quantity [Mol%]	QTY	TRUE	0.0000
Time [Min]	RT	FALSE	0.00
Area [uV.Min]	AREA	FALSE	0.00
Area [Norm]	AREAP	TRUE	0.0

Appendix B: Physical Constants

Identifier
MW
IGHV
INHV
SUMM_FACT
ZFACTOR
IRD
GASGALLIQ
LBS_GAL
MON
RON
ASTM_VP
REL_SENS

Appendix C: Report Families and Temperatures for Components

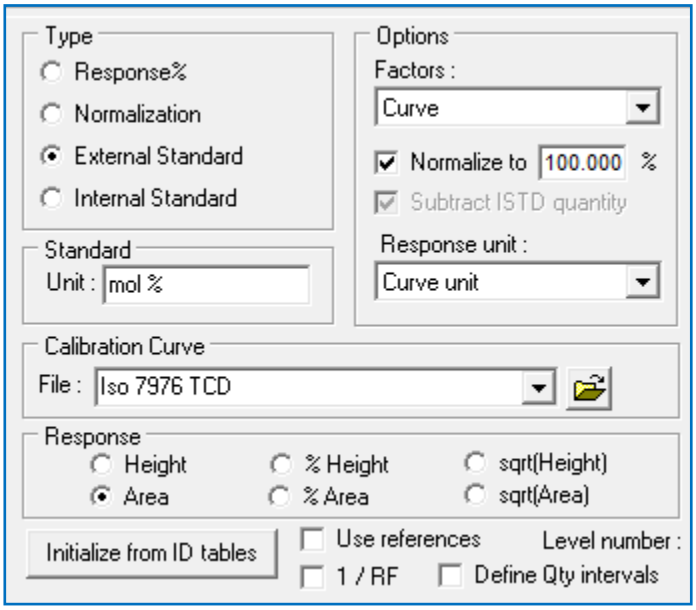
Name	Temperature
ISO	0 °C
ISO	15 °C
ISO	20 °C
ASTM	60 °F
GPA	60 °F

Appendix D: Report Families and Pressure for Calculations

Name	Pressure
ISO	101.325
ASTM	14.696
GPA	14.696
GPA	14.65
GPA	14.73
GPA	15.025

Appendix E: IS0 6976 Natural Gas – Calculation of Calorific Values, Density, Relative Density and Wobbe Index from Composition

CDS calculates natural gas component concentrations and reports these as non-normalized mole percent (Mol%). ISO-6976 requires that these data be presented as normalized to 100% and this is usually done by simply checking the normalized data checkbox in the Calibration section of the CompassCDS method prior to processing or re-processing the data as shown below.



By way of example, non-normalized results of a natural gas sample reflect a Quantity (QTY) total (in Mol%) of 95.09 as shown below

#	Name	Time [Min]	Quantity [mol %]	Height [µV]	Area [µV.Min]	Area % [%]
1	Nitrogen	0.20	2.37	23.7	0.5033	2.507
2	Methane	0.40	81.01	810.0	17.0950	85.162
3	Carbon Dioxide	0.60	2.54	25.4	0.5377	2.678
4	Ethane	0.80	1.81	18.2	0.3832	1.909
5	Propane	1.00	3.22	32.0	0.6789	3.382
6	i-Butane	1.20	2.10	21.0	0.4438	2.211
7	n-Butane	1.40	2.04	20.4	0.4317	2.150
Total			95.09	950.8	20.0735	100.000

Whereas, when the Normalize to 100% checkbox is selected, these same data reflect a QTY total of 100% as shown below

#	Name	Time [Min]	Quantity [%]	Height [µV]	Area [µV.Min]	Area % [%]
1	Nitrogen	0.20	2.49	23.7	0.5033	2.507
2	Methane	0.40	85.19	810.0	17.0950	85.162
3	Carbon Dioxide	0.60	2.67	25.4	0.5377	2.678
4	Ethane	0.80	1.90	18.2	0.3832	1.909
5	Propane	1.00	3.39	32.0	0.6789	3.382
6	i-Butane	1.20	2.21	21.0	0.4438	2.211
7	n-Butane	1.40	2.15	20.4	0.4317	2.150
Total			100.00	950.8	20.0735	100.000

This works in the case of single channel data as all of the results data being normalized to 100% are in the same channel. **However, in cases where results data are being obtained from more than 1 channel (e.g. FID/TCD) this option cannot be used as both channels would be independently normalized to 100% and the resultant normalized data would be incorrect as the combined QTY data set would not add up to 100%. In this case, the non-normalized results (QTY mol%) data from each channel would have to be combined and then normalized by the plug-in via a checkbox option [Normalize Results].**

Using CDS custom variables, this equation would be

(QTY/SUM('QTY'))*100

For the NatGas report the normalization of the QTY value requires the following equation

(QTY/SUM('QTY'))*100

which, when expanded means the quantity (in Mol%) of each identified and quantified component (which may be from several detector channels) is divided by the sum of the quantities of all of the identified components and then multiplied by 100. **These values must add up to 100.00 Mol%** Using the following data set as an example, the calculated results for GPA2172 are as follows:

Peak Name	RT [min]	Reported QTY Mol% (un-normalized)	
Nitrogen	0.2	2.37	(Ch1 TCD)
Methane	0.4	81.01	(Ch1 TCD)
Carbon Dioxide	0.6	2.54	(Ch1 TCD)
Ethane	0.8	1.81	(Ch2 FID)
Propane	1.0	3.22	(Ch2 FID)
i-Butane	1.2	2.10	(Ch2 FID)
n-Butane	1.4	2.04	(Ch2 FID)

To normalize these results the software would sum the QTY amounts shown above (100.7913) and then divide each one of the component amounts by this value and multiply by 100, for example:

For Nitrogen it would be (2.37/95.09)*100 = 2.4923

For Methane it would be (81.01/95.09)*100 = 85.1930

For Carbon Dioxide it would be (2.54/95.09)*100 = 2.6712

For Ethane it would be (1.81/95.09)*100 = 1.9035

For Propane it would be (3.22/95.09)*100 = 3.3863

For i-Butane it would be (2.10/95.09)*100 = 2.2084

For n-Butane it would be (2.04/95.09)*100 = 2.1453

These all add up to a total of 100 (Mol %) when normalized in this way. To get to this "starting point" of the calculation, the user should be able to select the components to be reported from a list of all natural gas components that uses standardized names. In this case he/she would have selected the list of components to be analyzed using the NatGas Results section of the Multi-Channel report plug-in. By clicking on the Component Selection dropdown list, each component to be analysed would be checked and the software would then know to find the un-normalized results for each of these components for a particular sample in the CompassCDS Database and normalize these (as shown above) as a first step.

These normalized results data represent the initial values that most of the following ISO-6967 calculations are based upon.

Once these data have been calculated and normalized, the plug-in will use values from one of four XML format data tables to calculate and (selectively) display the following:

1) Fraction Molecular Weight of each selected component
2) Fraction Molecular Weight Fraction Total (this is the calculated molecular weight of the sample based on composition)
3) Superior Calorific Value based on Molar basis
4) Inferior Calorific Value based on Molar basis
5) Superior Calorific Value based on Mass basis
6) Inferior Calorific Value based on Mass basis
7) Superior Calorific Value based on Volumetric basis
8) Inferior Calorific Value based on Volumetric basis
9) Compressibility
10) Ideal Gas Density
11) Real Gas Density
12) Ideal Relative Density
13) Real Relative Density
14) Wobbe Index

1) The first calculation is the **Fraction Molecular Weight** and

2) Molecular Weight Fraction Total or MW value. This calculation uses the molecular weight value associated with each component and the calculation is done as follows:

$$(QTY_{Component}/100) \times MW_{Component} = MW_{Fraction} \ldots\ldots\ldots\ldots \text{Equation 1}$$

In XML format this equation is expressed as:

ISO_MOLXMW = (QTY/100)*ISO_MW

Summation all the MW fractions provides the MW Total for the sample. Using the example data set above, the calculation of the MW results is done as follows:

Name	MW	QTY [Mol%]	Fraction MW
Nitrogen	28.0135	2.49	0.6975
Methane	16.043	85.19	13.6670
Carbon Dioxide	44.01	2.67	1.1751
Ethane	30.07	1.9	0.5713
Propane	44.097	3.39	1.4949
i-Butane	58.123	2.21	1.2845
n-Butane	58.123	2.15	1.2496
Total		**100**	**20.1400**

The fraction molecular weight calculation is independent of Temperature and Pressure i.e. is calculated only once for all T/Press regimes. In this example, the individual fraction molecular weight values would be displayed as a column in the peak results table and the Total of all of these would represent the reported sample or total molecular weight value which in this example is 21.1400

Once the Fraction MW values have been calculated, the next values to be determined are the **Calorific Values.** These values can be calculated and reported at pressure base of 101.325 kPa on a Molar ($kJ.mol^{-1}$), Mass ($Mj.kg^{-1}$) or Volumetric ($Mj.m^{-3}$) basis and at one of four temperatures 0°C, 15°C, 20°C and 25°C. These values are also reported as Superior or Inferior.

Superior calorific value is defined as:
T*he amount of heat which would be released by the complete combustion in air of a specified quantity of gas, ins such a way that the pressure p_1 at which the reaction takes place remains constant and all the products of combustion are returned to the same specified temperature t_1 as that of the reactants, all of these reactants being in a gaseous state except for water formed by the combustion which is condensed to the liquid state at t_1.*

Inferior calorific value is defined as:
T*he amount of heat which would be released by the complete combustion in air of a specified quantity of gas, ins such a way that the pressure p_1 at which the reaction takes place remains constant and all the products of combustion are returned to the same specified temperature t_1 as that of the reactants, all of these reactants being in a gaseous state.*

The general equation that define calorific value calculations is as follows:

To calculate these values on a Molar basis i.e. ($kJ.mol^{-1}$) from CompassCDS results data the equation would be:

$$H^{o}_{component} = ((QTY_{Component}/100)*HV_{component} \quad \ldots\ldots\ldots\ldots \text{ Equation 2}$$

In XML format this equation is expressed as:

3) For superior heating value:

$$ISO_SUPERIOR = ((QTY_{Component}/100)*ISO_IGHV)$$

4) For inferior heating value:

$$ISO_INFERIOR = ((QTY_{Component}/100)*ISO_INHV)$$

Where $QTY_{Component}$ is the calculated quantity fraction of the component and $HV_{component}$ is the superior or inferior calorific heating value of that component a specific temperature, obtained from the accompanying tables. Summation of the calculated component molar calorific heating value provide the total molar heating value reported in $kJ.mol^{-1}$ and there would be a Superior and Inferior value reported. By way of example using the data from above, the molar calorific heating value for the mixture at 25 ^{o}C would be:

Name	MW	QTY [Mol%]	Fraction MW	Ideal HV Sup	Ideal HV Inf	Superior HV (kJ.mol-1)	Inferior HV (kJ.mol-1)
Nitrogen	28.0135	2.49	0.6975	0	0	0.000	0.000
Methane	16.043	85.19	13.6670	890.6300	802.600	758.728	683.735
Carbon Dioxide	44.01	2.67	1.1751	0	0	0.000	0.000
Ethane	30.07	1.9	0.5713	1560.690	1428.640	29.653	27.144
Propane	44.097	3.39	1.4949	2219.170	2043.110	75.230	69.261
i-Butane	58.123	2.21	1.2845	2868.200	2648.120	63.387	58.523
n-Butane	58.123	2.15	1.2496	2877.400	2657.320	61.864	57.132
Total		**100**	**20.1400**			**988.862**	**895.796**

To calculate the molar calorific heating values at 20, 15 and 0^{o}C the ideal superior and inferior 25^{o}C heating values are simply substituted with the corresponding ones in the table.

To calculate the calorific heating values based on mass ($MJ.kg^{-1}$) the following equation is used

5) For superior heating value:

$$ISO_CVPERKGS = SUM('ISO_SUPERIOR')/SUM('ISO_MOLXMW')$$

6) For Inferior heating value:

$$ISO_CVPERKGI = SUM('ISO_INFERIOR')/SUM('ISO_MOLXMW')$$

Using the values calculated in the previous example, the Superior and Inferior calorific heating values are 988.682 & 895.796 $kJ.mol^{-1}$ respectively and the mixture molecular weight is 20.14.

Therefore, to calculate the mass based calorific heating values:

Superior HV = 988.682/20.14 = 49.090 ($MJ.kg^{-1}$)

Inferior HV = 895.796/20.14 = 44.478 ($MJ.kg^{-1}$)

To calculate the calorific heating values based on volume (MJ.m^{-3}) the following equation is used

7) For superior heating value:

ISO_CVPERCMS = (SUM('ISO_SUPERIOR')*101.325)/(288.15*8.314510)

8) For inferior heating value:

ISO_CVPERCMI = (SUM('ISO_INFERIOR')*101.325)/(288.15*8.314510)

Where R = Molar gas constant 8.314510 J.mol^{-1}K^{-1}

P_2 is the pressure 101.325 kPa

T is the measurement temperature in Kelvins 15^{o}C = 288.15

Using the values calculated in the first (kJ.mol^{-1}) example, the Superior and Inferior calorific heating values are 988.682 & 895.796 kJ.mol^{-1}

Therefore to calculate the volume based calorific heating values:

ISO_CVPERCMS = (988.682*101.325)/(288.15*8.314510) = 100178.2/2395.826 = 41.8136 (MJ.m^{-3})

ISO_CVPERCMI = (895.796*101.325)/(288.15*8.314510) = 90766.529/2395.826 = 37.8853 (MJ.m^{-3})

9) Calculation of Compression Factor: This calculation uses the following equation to calculate the compression factor:

In order to calculate the Compression Factor or Compressibility, the individual component compressibility values have to first be calculated using the following equation:

ISO_COMP_COMP = (QTY/100)*ISO_SUMM_FACT

Where ISO_SUMM_FACT is the summation factor provided for each component and QTY is the normalized quantity of each component.

Name	MW	QTY [Mol%]	Fraction MW	Summation 15^{o}C	Component Compressibility
Nitrogen	28.0135	2.49	0.6975	0.0173	0.00043
Methane	16.043	85.19	13.6670	0.0447	0.03808
Carbon Dioxide	44.01	2.67	1.1751	0.0748	0.00200
Ethane	30.07	1.9	0.5713	0.0922	0.00175
Propane	44.097	3.39	1.4949	0.1338	0.00454
i-Butane	58.123	2.21	1.2845	0.1789	0.00395
n-Butane	58.123	2.15	1.2496	0.1871	0.00402
Total		**100**	**20.1400**		**0.05477**

Sum of individual component compressibilities is 0.05477

Therefore, sample compressibility factor is calculated using the following equation:

ISO_COMP_SAMP = 1-SQR(SUM('ISO_COMP_COMP'))

Using the example above the compressibility of this mixture at 15^0C would be:

ISO_COMP_SAMP = 1 – (0.05477 *0.05477) = 1 – 0.0029997 = 0.997

In order to Calculate Relative Density, the Fractional Relative Density for each component has to be calculated using the following equation:

$$ISO_PEAK_IRD = (QTY_{Component}/100)*ISO_MW$$

Where $QTY_{Component}$ is the normalized amount of the component and ISO_MW is the molecular weight of that component. The example below shows this calculation.

Name	MW	QTY [Mol%]	ISO_PEAK_IRD
Nitrogen	28.0135	2.49	0.6975
Methane	16.043	85.19	13.6670
Carbon Dioxide	44.01	2.67	1.1751
Ethane	30.07	1.9	0.5713
Propane	44.097	3.39	1.4949
i-Butane	58.123	2.21	1.2845
n-Butane	58.123	2.15	1.2496
Total		**100**	**20.1400**

10) Ideal Gas Density is then calculated using the following equation:

ISO_IGD = SUM('ISO_PEAK_IRD')*(ISO_PRESSBASE/(8.314510*288.15))

Where pressure base is 101.325 kPa therefore

ISO_IGD = SUM(20.1400)*(101.325/(8.314510*288.15)) = 0.8517

11) Real Gas Density is calculated as follows:

ISO_IRG = ISO_IGD/ISO_COMP_SAMP

ISO_IRG = 0.8517/0.997 = 0.8543

12) Ideal Relative Density is calculated as follows:

ISO_IRD = SUM('ISO_PEAK_IRD')/28.9626

Where 28.9626 = density of air

ISO_IRD = 20.14/28.9626 = 0.6953

13) Real Relative Density is calculated as follows:

ISO_RRD = ISO_IRD*(ISO_COMP_AIR/ISO_COMP_SAMP)

Where ISO_COMP_AIR = Compressibilty of Air = 0.99958 and ISO_COMP_SAMP = Compressibility of sample (in above example = 0.997

ISO_RRD = 0.6953*(0.99958/0.997) = 0.6970

14) Wobbe Index is calculated as follows:

ISO_WOBBE = ISO_CVPERCMS/SQRT(ISO_IRD)

ISO_WOBBE = 41.8136/SQRT(0.6953) = 50.1458